

AMENDMENTS TO THE SPECIFICATION

IN THE SPECIFICATION:

Please replace the paragraph on page 14, lines 11-23 with the following rewritten paragraph:

Referring to FIG. 6, ~~an example of a predetermined~~ the inventive angle dividing rule (ADR) will be described below. In the angle dividing rule adopted herein, an angle of 360 degrees is divided into 12 angular ranges in the form of a clock dial. To the center of each of the divided angular ranges, a symbol corresponding to a figure of the clock dial is added. As shown in FIG. 6, 12 angular symbols including ze (zero), on (one), tw (two), th (three), fo (four), fi (five), si (six), se (seven), ei (eight), ni (nine), te (ten) and el (eleven) are provided in the angular ranges of one o'clock, two o'clock, three o'clock, four o'clock, five o'clock, six o'clock, seven o'clock, eight o'clock, nine o'clock, ten o'clock and eleven o'clock, respectively. By these 12 angular symbols, corresponding angular ranges are expressed.

Please replace the paragraph on page 15, lines 9-12 with the following rewritten paragraph:

According to the ~~angle-dividing rule~~ (ADR) shown in FIG. 6, on the basis of information on the molecular three-dimensional structure of  $\alpha$ -Glc-4C, an angular symbol "si" is given to the above described noticed "Q1" 11 in level 4.

AMENDMENTS TO THE CLAIMS

1. (Currently Amended) A molecular stereochemical coding computer program containing program instructions executable by a computer and ~~capable of~~ causing said computer to take a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, said instructions comprising:

classifying atoms in a hierarchy by assigning a start atom, ~~which is to be coded,~~ to a zero-th hierarchical level as the lowest hierarchy, assigning ~~another atom, which is~~ all atoms which are directly bonded to said start atom to a first hierarchical level, assigning ~~an atom, which is~~ all atoms, except said start atom, which are bonded to said ~~another atom~~ atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly, sequentially assigning atoms to hierarchical levels until a final hierarchy is made in a form which may be accessed by a processor;

forming a molecular tree with a precedence rule by placing said atoms, which belong to the same hierarchical level, in an order in accordance with said precedence rule to form a said molecular tree wherein ~~every~~ said start atom from a lower hierarchical level to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms;

coding one atom, which was assigned to ~~the~~ a (n+3)-th hierarchical level, wherein n is an integer of 0 or more, in said

molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the  $(n+3)$ -th hierarchical level, an atom in ~~the~~ a  $(n+2)$ -th hierarchical level and an atom in ~~the~~ a  $(n+1)$ -th hierarchical level, and a theoretical plane, which is formed by the atom in the  $(n+2)$ -th hierarchical level, the atom in the  $(n+1)$ -th hierarchical level and an atom in ~~the~~ a  $n$ -th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the  $(n+3)$ -th hierarchical level, the atom in the  $(n+2)$ -th hierarchical level which is bonded to the atom in the  $(n+3)$ -th hierarchical level, the atom in the  $(n+1)$ -th hierarchical level which is bonded to the atom in the  $(n+2)$ -th hierarchical level, and the atom in the  $n$ -th hierarchical level which is bonded to the atom in the  $(n+1)$ -th hierarchical level, replacing the derived dihedral angle with an angular symbol in accordance with an angle dividing rule (ADR) based on the magnitude of the dihedral angle, assigning the angular symbol to the coded atom in the  $(n+3)$ -th hierarchical level, and similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; ~~and~~

with a linear notation rule, expressing said molecular tree by a row of characters, carrying out linear notation of a set of angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree, preparing a conformation code

indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms; and

further comprising printing or recording the conformation code of the molecule on computer readable recording media.

2. (Currently Amended) The computer program as set forth in claim 1, which further comprises instructions for preparing a configuration code indicative of a configuration of the molecule for every said start atom, and

coding an atom in the n-th hierarchical level by assigning said atom as a reference position, integrally rotating all of the atoms belonging to the (n+3)-th hierarchical level around a bonding axis, which connects the atom in the (n+1)-th hierarchical level to the atom in the (n+2)-th hierarchical level, so that an atom, which has precedence in accordance with said precedence rule among said atoms belonging to the (n+3)-th hierarchical level, is positioned at an angular position with respect to said reference position, giving an angular symbol according to said ~~angle-dividing-rule~~ ADR to each of said atoms belonging to the (n+3)-th hierarchical level, in accordance with an angular position after rotation with respect to said reference position, carrying out the linear notation of a set of said plurality of angular symbols in accordance with said

linear notation rule so as to correspond to said molecular tree, and ~~prepare~~ preparing a configuration code for every said start atom.

3. (Currently Amended) The computer program as set forth in claim 1 or 2, which further comprises instructions for preparing a planar structure code indicative of a planar structure of the molecule for every said start atom,

wherein said molecular tree is expressed by a set of planar structure symbols which planar-structurally express a bonding relationship between said plurality of atoms, carrying out the linear notation of said set of planar structure symbols in accordance with said linear notation rule so as to correspond to said molecular tree, preparing a planar structure code indicative of the planar structure of the molecule with respect to said start atom, and similarly, preparing planar structure codes with respect to other start atoms.

4. (Previously Presented) The computer program as set forth in claim 3, wherein said conformation codes, said configuration codes and said planar structure codes are expressed in parallel with respect to said start atoms.

5. (Currently Amended) The computer program as set forth in claim 2, wherein when it is impossible to rotate said atoms belonging to the (n+3)-th hierarchical level around the bonding axis connecting the atom belonging to the (n+1)-th hierarchical level to the atom belonging to the (n+2)-th hierarchical level, said angular symbols given at said coding step are adopted as they are, and the linear notation of a set of said plurality of angular symbols is carried out in accordance with said linear notation rule so as to correspond to said molecular tree, to prepare said configuration codes for every said start atom.

6. (Previously Presented) The computer program as set forth in claim 3, wherein said planar structural codes are CANOST linear notations.

7. (Previously Presented) The computer program as set forth in claim 1, wherein said precedence rule is a CANOST code precedence rule.

8. (Previously Presented) The computer program as set forth in claim 1, wherein said linear notation rule is a CANOST code linear notation rule.

9. (Previously Presented) The computer program as set forth in claim 1, wherein during the formation of said molecular tree, a group of atoms having a low degree of coding in the identification of stereochemistry are replaced with symbols to be masked.

10. (Currently Amended) The computer program as set forth in claim 1, wherein said ~~angle-dividing rule~~ ADR divides an angle of 360 degrees into a number of clock-dial-like angular ranges, and the divided angular ranges are reflected in the level of abundance to be unequally divided.

11. (Previously Presented) The computer program as set forth in claim 1, wherein during the preparation of said conformation codes, said conformation codes are prepared with respect to at least two of said start atoms, the hierarchical level numbers of which are spaced from each other by three hierarchical levels or more.

12. (Cancelled)

13. (Currently Amended) A computer readable medium containing instructions, executed by a processor, for performing a method for taking a stereochemistry about each of a plurality of atoms



constituting a molecule to code the molecule, said method comprising:

classifying atoms in a hierarchy by assigning a start atom, ~~which is to be coded,~~ to a zero-th hierarchical level as the lowest hierarchy, assigning ~~another atom, which is~~ all atoms which are directly bonded to said start atom to a first hierarchical level, assigning ~~an atom, which is~~ all atoms, except said start atom, which are bonded to said ~~another atom~~ atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly, sequentially assigning atoms to hierarchical levels until a final hierarchy is made in a form which may be accessed;

forming a molecular tree with a precedence rule by placing said atoms, which belong to the same hierarchical level, in an order in accordance with said precedence rule to form a molecular tree wherein every said start atom from a lower hierarchical level to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms;

coding one atom, which was assigned to ~~the~~ a (n+3)-th hierarchical level, wherein n is an integer of 0 or more, in said molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the (n+3)-th hierarchical level, an atom in ~~the~~ a (n+2)-th hierarchical level and an atom in ~~the~~ a (n+1)-th hierarchical level, and a theoretical plane, which

is formed by the atom in the (n+2)-th hierarchical level, the atom in the (n+1)-th hierarchical level and an atom in the a n-th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the (n+3)-th hierarchical level, the atom in the (n+2)-th hierarchical level which is bonded to the atom in the (n+3)-th hierarchical level, the atom in the (n+1)-th hierarchical level which is bonded to the atom in the (n+2)-th hierarchical level, and the atom in the n-th hierarchical level which is bonded to the atom in the (n+1)-th hierarchical level, replacing the derived dihedral angle with an angular symbol in accordance with an angle dividing rule (ADR) based on the magnitude of the dihedral angle, assigning the angular symbol to the coded atom in the (n+3)-th hierarchical level, and similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; and

with a linear notation rule, expressing said molecular tree by a row of characters, carrying out linear notation of a set of angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms,

wherein the codes of the molecule are recorded in a computer

readable recording medium to give the stereochemistry about each of a plurality of atoms constituting the molecule.

14. (Previously Presented) The computer program as set forth in claim 1, further comprising calculating NMR shifts based upon said conformation codes.

15. (Previously Presented) The computer program as set forth in claim 14, wherein the NMR shifts are printed on computer readable recording media.

16. (Currently amended) The computer program as set forth in claim 2, further comprising printing or recording the ~~conformation code~~ and configuration code of the molecule on computer readable recording media.

17. (Cancelled)

18. (New) A method for taking a stereochemistry about each of a plurality of atoms constituting a molecule to code the molecule, said method comprising:

classifying atoms in a hierarchy by assigning a start atom to a zero-th hierarchical level as the lowest hierarchy, assigning all

atoms which are directly bonded to said start atom to a first hierarchical level, assigning all atoms, except said start atom, which are bonded to said atoms assigned to said first hierarchical level, to a second hierarchical level, and similarly, sequentially assigning atoms to hierarchical levels until a final hierarchy is made in a form which may be accessed;

forming a molecular tree with a precedence rule by placing said atoms, which belong to the same hierarchical level, in an order in accordance with said precedence rule to form a molecular tree wherein said start atom from a lower hierarchical level to a higher hierarchical level is expressed in a bonding relationship between said plurality of atoms;

coding one atom, which was assigned to a  $(n+3)$ -th hierarchical level, wherein  $n$  is an integer of 0 or more, in said molecular tree, by deriving a dihedral angle between a theoretical plane, which is formed by an atom in the  $(n+3)$ -th hierarchical level, an atom in a  $(n+2)$ -th hierarchical level and an atom in a  $(n+1)$ -th hierarchical level, and a plane, which is formed by the atom in the  $(n+2)$ -th hierarchical level, the atom in the  $(n+1)$ -th hierarchical level and an atom in a  $n$ -th hierarchical level, with respect to a group comprising four atoms which consists of said coded atom in the  $(n+3)$ -th hierarchical level, the atom in the  $(n+2)$ -th hierarchical level which is bonded to the atom in the  $(n+3)$ -th

hierarchical level, the atom in the (n+1)-th hierarchical level which is bonded to the atom in the (n+2)-th hierarchical level, and the atom in the n-th hierarchical level which is bonded to the atom in the (n+1)-th hierarchical level, replacing the derived dihedral angle with an angular symbol in accordance with an angle dividing rule ADR based on the magnitude of the dihedral angle, assigning the angular symbol to the coded atom in the (n+3)-th hierarchical level, and similarly, assigning angular symbols based on the magnitudes of dihedral angles with respect to other atoms to be coded; and

with a linear notation rule, expressing said molecular tree by a row of characters, carrying out linear notation of a set of angular symbols in accordance with said linear notation rule so as to correspond to said molecular tree, preparing a conformation code indicative of a conformation of the molecule with respect to said start atom, and similarly, preparing conformation codes with respect to other start atoms.